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DOPING BiI_3 : A COMPUTATIONAL STUDY OF ELECTRONIC PROPERTIES

Yvette Anguiano

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Bismuth tri-iodide (BiI_3) has recently been proposed as a photovoltaic material. However, in order to improve the efficiency of BiI_3 based photovoltaics, suitable dopants need to be identified. We have used density functional theory calculations to study the electronic properties of BiI_3 with substituent dopants at either the bismuth or the iodine site. Based on the density of states calculations, we predict, Ti and Zr are potential *n*-type dopants substituting Bi with contributions to the conduction band minimum and Ni is a potential *p*-type candidate with contributions to the valence band maximum. For substitution at the iodine site, we examined Sb and Te, and they were found to be suitable *p*-type dopants.